



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:35 PM EDT

PDB ID : 3EH5 / pdb_00003eh5
Title : Structure of the reduced form of cytochrome ba3 oxidase from *Thermus thermophilus*
Authors : Liu, B.; Chen, Y.; Doukov, T.; Soltis, S.M.; Stout, D.; Fee, J.A.
Deposited on : 2008-09-11
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

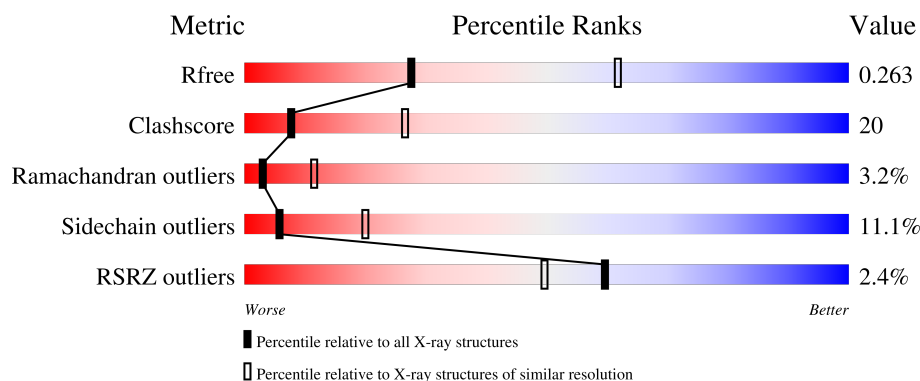
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	618	2% 52% 31% 6% 10%
2	B	166	% 64% 28% 8%
3	C	33	3% 73% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HAS	A	801	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	4409	2985	709	699	16	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-55	SER	-	expression tag	UNP Q5SJ79
A	-54	GLU	-	expression tag	UNP Q5SJ79
A	-53	ILE	-	expression tag	UNP Q5SJ79
A	-52	SER	-	expression tag	UNP Q5SJ79
A	-51	ARG	-	expression tag	UNP Q5SJ79
A	-50	VAL	-	expression tag	UNP Q5SJ79
A	-49	TYR	-	expression tag	UNP Q5SJ79
A	-48	GLU	-	expression tag	UNP Q5SJ79
A	-47	ALA	-	expression tag	UNP Q5SJ79
A	-46	TYR	-	expression tag	UNP Q5SJ79
A	-45	PRO	-	expression tag	UNP Q5SJ79
A	-44	GLU	-	expression tag	UNP Q5SJ79
A	-43	LYS	-	expression tag	UNP Q5SJ79
A	-42	LYS	-	expression tag	UNP Q5SJ79
A	-41	ALA	-	expression tag	UNP Q5SJ79
A	-40	THR	-	expression tag	UNP Q5SJ79
A	-39	LEU	-	expression tag	UNP Q5SJ79
A	-38	TYR	-	expression tag	UNP Q5SJ79
A	-37	PHE	-	expression tag	UNP Q5SJ79
A	-36	LEU	-	expression tag	UNP Q5SJ79
A	-35	VAL	-	expression tag	UNP Q5SJ79
A	-34	LEU	-	expression tag	UNP Q5SJ79
A	-33	GLY	-	expression tag	UNP Q5SJ79
A	-32	PHE	-	expression tag	UNP Q5SJ79
A	-31	LEU	-	expression tag	UNP Q5SJ79
A	-30	ALA	-	expression tag	UNP Q5SJ79
A	-29	LEU	-	expression tag	UNP Q5SJ79

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	ILE	-	expression tag	UNP Q5SJ79
A	-27	VAL	-	expression tag	UNP Q5SJ79
A	-26	GLY	-	expression tag	UNP Q5SJ79
A	-25	SER	-	expression tag	UNP Q5SJ79
A	-24	LEU	-	expression tag	UNP Q5SJ79
A	-23	PHE	-	expression tag	UNP Q5SJ79
A	-22	GLY	-	expression tag	UNP Q5SJ79
A	-21	PRO	-	expression tag	UNP Q5SJ79
A	-20	PHE	-	expression tag	UNP Q5SJ79
A	-19	GLN	-	expression tag	UNP Q5SJ79
A	-18	ALA	-	expression tag	UNP Q5SJ79
A	-17	LEU	-	expression tag	UNP Q5SJ79
A	-16	ASN	-	expression tag	UNP Q5SJ79
A	-15	TYR	-	expression tag	UNP Q5SJ79
A	-14	GLY	-	expression tag	UNP Q5SJ79
A	-13	ASN	-	expression tag	UNP Q5SJ79
A	-12	VAL	-	expression tag	UNP Q5SJ79
A	-11	ASP	-	expression tag	UNP Q5SJ79
A	-10	ALA	-	expression tag	UNP Q5SJ79
A	-9	TYR	-	expression tag	UNP Q5SJ79
A	-8	PRO	-	expression tag	UNP Q5SJ79
A	-7	LEU	-	expression tag	UNP Q5SJ79
A	-6	LEU	-	expression tag	UNP Q5SJ79
A	-5	MET	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79
A	258	ARG	LYS	engineered mutation	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	217	233	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	engineered mutation	UNP Q5SJ80

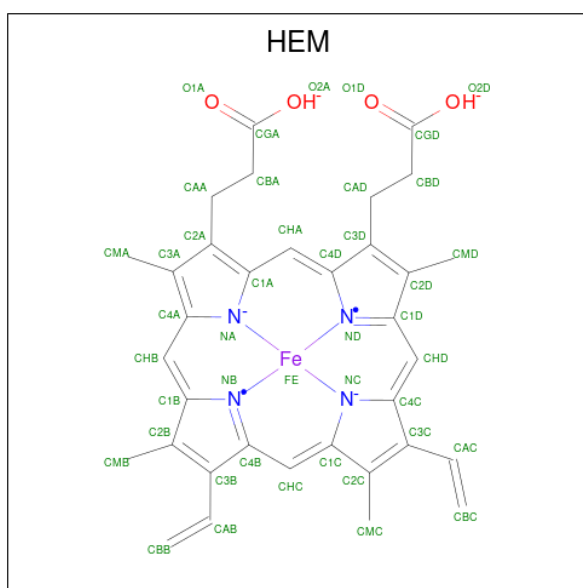
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

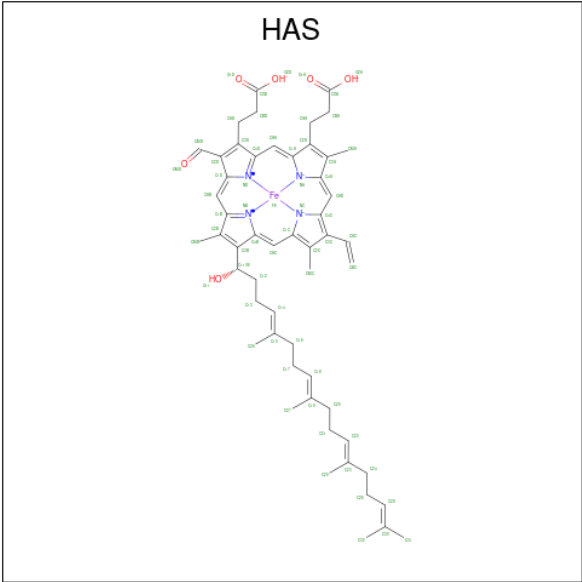
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



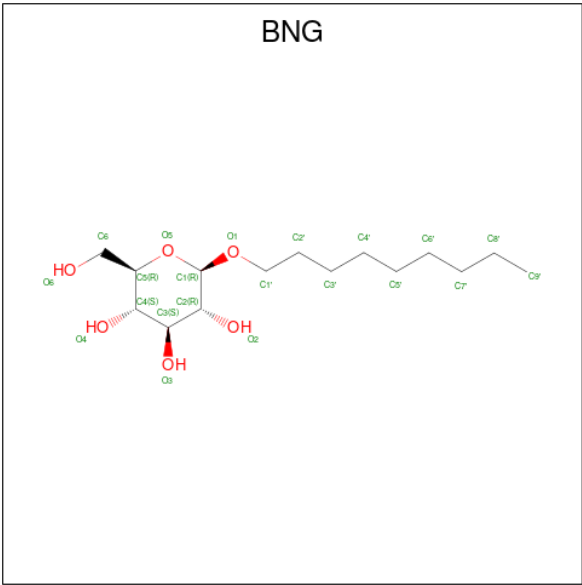
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula: $\text{C}_{54}\text{H}_{64}\text{FeN}_4\text{O}_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Fe	N	O	
6	A	1	65	54	1	4	6	0

- Molecule 7 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



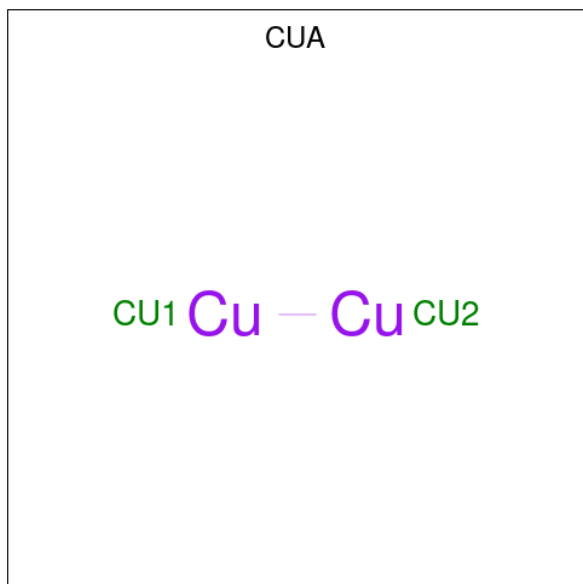
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	21	15	6	0	0
7	A	1	21	15	6	0	0
7	A	1	21	15	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			21	15	6		

- Molecule 8 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cu	0	0
			2	2		

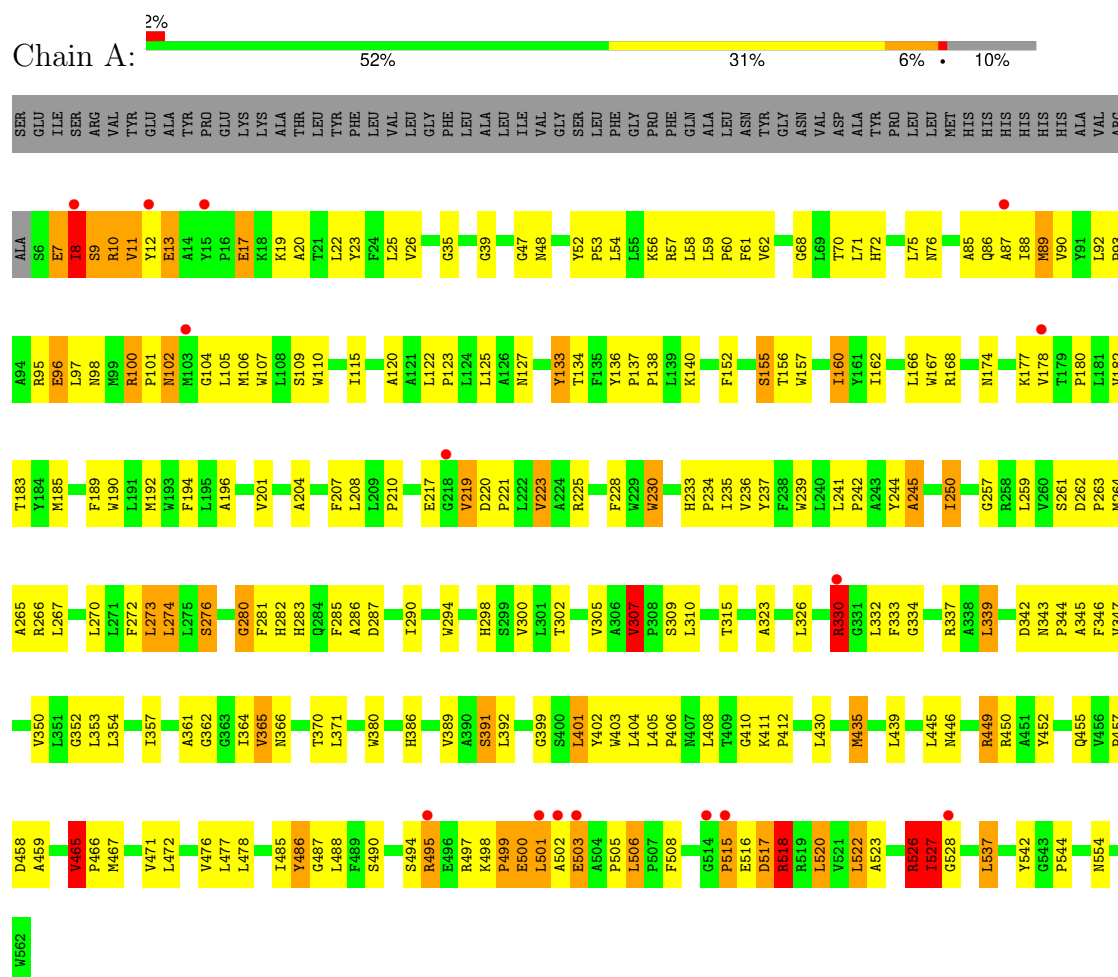
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	63	Total	O	0	0
			63	63		
9	B	19	Total	O	0	0
			19	19		
9	C	1	Total	O	0	0
			1	1		

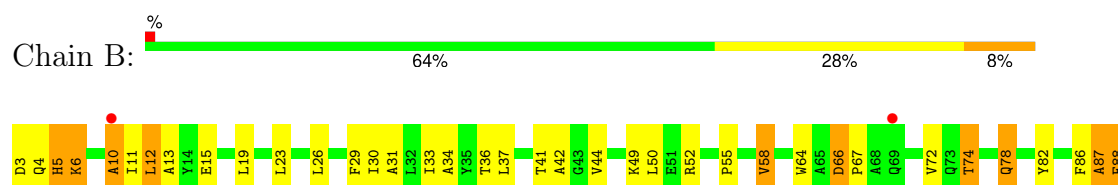
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome c oxidase subunit 1

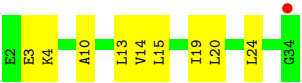


• Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 3: Cytochrome c oxidase polypeptide 2A



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.63Å 115.63Å 149.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.80) 99.4 (20.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.257 0.198 , 0.263	Depositor DCC
R_{free} test set	1689 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 112.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6244	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HAS, BNG, HEM, CUA, CU1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.13	9/4566 (0.2%)	1.28	27/6266 (0.4%)
2	B	1.16	4/1335 (0.3%)	1.27	6/1822 (0.3%)
3	C	1.22	0/265	1.21	0/359
All	All	1.14	13/6166 (0.2%)	1.28	33/8447 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	VAL	CA-CB	8.19	1.63	1.54
2	B	97	VAL	C-O	-7.34	1.19	1.24
1	A	137	PRO	CA-C	7.14	1.55	1.51
1	A	307	VAL	CA-CB	7.00	1.58	1.54
1	A	286	ALA	CA-CB	-6.40	1.44	1.53
1	A	357	ILE	CA-C	5.42	1.58	1.52
1	A	115	ILE	CA-CB	5.41	1.60	1.54
2	B	118	VAL	CA-CB	5.40	1.60	1.53
1	A	361	ALA	CA-C	5.34	1.59	1.52
1	A	365	VAL	CA-C	5.09	1.58	1.52
2	B	107	ILE	CA-C	-5.08	1.46	1.52
2	B	72	VAL	CA-CB	5.05	1.60	1.54
1	A	476	VAL	CA-CB	5.05	1.60	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	ASP	CA-C-N	9.07	131.18	119.84
2	B	66	ASP	C-N-CA	9.07	131.18	119.84
1	A	465	VAL	CA-C-N	-8.91	110.47	119.56
1	A	465	VAL	C-N-CA	-8.91	110.47	119.56
2	B	58	VAL	N-CA-C	7.71	118.48	110.62
1	A	9	SER	N-CA-C	-7.67	98.82	110.70
1	A	223	VAL	N-CA-CB	7.41	118.73	110.51
1	A	230	TRP	N-CA-C	-6.71	103.89	111.07
1	A	527	ILE	N-CA-C	6.69	116.71	110.42
1	A	39	GLY	CA-C-N	6.42	125.99	119.19
1	A	39	GLY	C-N-CA	6.42	125.99	119.19
2	B	146	ARG	CB-CG-CD	-6.36	96.67	111.30
1	A	503	GLU	N-CA-C	-6.26	101.50	111.02
1	A	435	MET	CG-SD-CE	6.22	114.58	100.90
1	A	261	SER	N-CA-C	6.19	118.15	107.93
1	A	273	LEU	N-CA-C	6.04	117.86	111.28
2	B	5	HIS	N-CA-C	-5.97	107.81	114.62
1	A	201	VAL	N-CA-C	5.69	116.42	110.62
1	A	100	ARG	CA-C-N	-5.56	114.20	119.76
1	A	100	ARG	C-N-CA	-5.56	114.20	119.76
1	A	537	LEU	N-CA-C	5.55	117.01	111.07
1	A	261	SER	CA-C-N	5.54	125.98	119.83
1	A	261	SER	C-N-CA	5.54	125.98	119.83
1	A	499	PRO	N-CA-C	5.50	123.81	112.47
1	A	500	GLU	N-CA-C	-5.45	104.75	111.40
1	A	10	ARG	N-CA-C	-5.41	106.38	112.87
1	A	353	LEU	CA-C-N	5.33	127.69	120.65
1	A	353	LEU	C-N-CA	5.33	127.69	120.65
1	A	236	VAL	N-CA-C	-5.31	105.22	111.00
1	A	245	ALA	N-CA-C	-5.22	105.23	111.03
2	B	72	VAL	CB-CA-C	5.19	116.32	110.41
1	A	380	TRP	N-CA-C	-5.18	105.71	111.36
1	A	488	LEU	N-CA-C	-5.17	105.54	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	503	GLU	Peptide
1	A	8	ILE	Peptide
2	B	87	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4409	0	4516	210	1
2	B	1298	0	1282	43	0
3	C	259	0	279	5	0
4	A	1	0	0	0	0
5	A	43	0	30	6	0
6	A	65	0	61	9	0
7	A	63	0	90	2	0
7	C	21	0	30	0	0
8	B	2	0	0	0	0
9	A	63	0	0	47	1
9	B	19	0	0	7	0
9	C	1	0	0	0	0
All	All	6244	0	6288	249	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.73	1.30
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.80	1.29
1:A:281:PHE:HD2	9:A:572:HOH:O	1.18	1.23
1:A:185:MET:HE1	9:A:624:HOH:O	1.04	1.19
1:A:273:LEU:HD12	9:A:607:HOH:O	1.46	1.15
1:A:506:LEU:H	1:A:506:LEU:HD23	1.14	1.13
1:A:93:PRO:HA	9:A:625:HOH:O	1.54	1.06
1:A:281:PHE:CD2	9:A:572:HOH:O	1.95	1.03
1:A:265:ALA:HB1	9:A:624:HOH:O	1.57	1.03
1:A:554:ASN:HD22	2:B:52:ARG:HG3	1.24	1.00
1:A:7:GLU:O	1:A:10:ARG:HG2	1.62	1.00
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.87	0.90
1:A:330:ARG:HH21	1:A:330:ARG:HG3	1.39	0.88
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.90	0.86
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.64	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LEU:HD23	1:A:506:LEU:N	1.86	0.86
1:A:410:GLY:HA3	1:A:499:PRO:HG3	1.57	0.85
1:A:22:LEU:O	1:A:26:VAL:HG23	1.76	0.84
1:A:96:GLU:HG2	9:A:625:HOH:O	1.77	0.84
1:A:109:SER:CB	9:A:614:HOH:O	2.27	0.81
1:A:445:LEU:O	1:A:446:ASN:HB2	1.80	0.80
1:A:500:GLU:HG2	1:A:501:LEU:H	1.46	0.80
1:A:554:ASN:ND2	2:B:52:ARG:HG3	1.96	0.80
1:A:20:ALA:HB3	1:A:106:MET:HE2	1.64	0.80
1:A:389:VAL:HG23	9:A:621:HOH:O	1.82	0.79
1:A:499:PRO:HB3	1:A:502:ALA:HB3	1.63	0.78
1:A:109:SER:HB3	9:A:614:HOH:O	1.81	0.78
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.70	0.77
1:A:520:LEU:HB2	9:A:617:HOH:O	1.84	0.76
2:B:101:ALA:O	2:B:103:ILE:HD12	1.84	0.76
1:A:86:GLN:HE22	1:A:155:SER:HB3	1.52	0.75
1:A:138:PRO:HB3	9:A:584:HOH:O	1.87	0.74
1:A:185:MET:CE	9:A:624:HOH:O	1.84	0.74
1:A:520:LEU:CB	9:A:617:HOH:O	2.34	0.74
1:A:505:PRO:HB3	9:A:594:HOH:O	1.88	0.73
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.02	0.73
2:B:142:PRO:HA	2:B:166:VAL:HG22	1.70	0.73
1:A:389:VAL:HB	6:A:801:HAS:HBC2	1.72	0.72
2:B:3:ASP:N	2:B:6:LYS:HB3	2.05	0.72
1:A:7:GLU:O	1:A:10:ARG:CG	2.38	0.71
1:A:497:ARG:C	1:A:499:PRO:HD3	2.15	0.71
1:A:228:PHE:HB3	9:A:568:HOH:O	1.90	0.70
1:A:352:GLY:C	1:A:392:LEU:HD13	2.17	0.70
1:A:523:ALA:O	1:A:526:ARG:HB2	1.92	0.70
1:A:59:LEU:HD22	1:A:61:PHE:HE1	1.56	0.69
1:A:167:TRP:HE3	9:A:616:HOH:O	1.77	0.67
1:A:192:MET:CB	9:A:607:HOH:O	2.42	0.67
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.11	0.66
1:A:273:LEU:HA	9:A:607:HOH:O	1.95	0.66
1:A:302:THR:O	1:A:305:VAL:HG12	1.97	0.65
2:B:148:ILE:HG22	9:B:181:HOH:O	1.96	0.65
1:A:217:GLU:O	9:A:587:HOH:O	2.15	0.64
1:A:125:LEU:HD22	9:A:578:HOH:O	1.96	0.64
1:A:264:MET:SD	2:B:15:GLU:HG2	2.37	0.64
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.81	0.63
1:A:52:TYR:N	1:A:53:PRO:HD2	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD21	1:A:180:PRO:HG2	1.80	0.62
2:B:134:THR:HG22	9:B:183:HOH:O	1.99	0.62
1:A:19:LYS:HG2	1:A:107:TRP:HZ2	1.64	0.62
1:A:330:ARG:HH21	1:A:330:ARG:CG	2.11	0.62
1:A:410:GLY:HA3	1:A:499:PRO:CG	2.30	0.62
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.82	0.61
2:B:86:PHE:O	2:B:88:PHE:N	2.32	0.61
1:A:498:LYS:N	1:A:499:PRO:HD3	2.15	0.61
2:B:142:PRO:HA	2:B:166:VAL:CG2	2.30	0.61
1:A:410:GLY:HA2	1:A:502:ALA:HB2	1.83	0.61
1:A:300:VAL:HG22	2:B:30:ILE:HD13	1.82	0.60
1:A:500:GLU:HG2	1:A:501:LEU:N	2.12	0.60
1:A:391:SER:HB3	9:A:577:HOH:O	2.00	0.60
1:A:120:ALA:O	1:A:123:PRO:HD2	2.00	0.60
1:A:402:TYR:N	1:A:402:TYR:CD2	2.69	0.60
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.83	0.60
1:A:506:LEU:H	1:A:506:LEU:CD2	1.84	0.60
3:C:15:LEU:O	3:C:19:ILE:HG13	2.02	0.59
1:A:404:LEU:HG	1:A:408:LEU:HD11	1.85	0.59
2:B:3:ASP:O	2:B:4:GLN:HB3	2.03	0.59
1:A:104:GLY:HA2	7:A:805:BNG:H4	1.85	0.58
1:A:140:LYS:NZ	9:A:593:HOH:O	2.36	0.58
1:A:237:TYR:O	1:A:241:LEU:HD13	2.02	0.58
1:A:182:VAL:HG21	1:A:508:PHE:CE2	2.38	0.58
2:B:74:THR:CG2	2:B:78:GLN:OE1	2.52	0.57
1:A:281:PHE:H	1:A:298:HIS:HD2	1.51	0.57
1:A:59:LEU:HD22	1:A:61:PHE:CE1	2.39	0.57
1:A:267:LEU:HD13	9:A:618:HOH:O	2.05	0.57
1:A:270:LEU:HD23	9:A:618:HOH:O	2.03	0.57
1:A:345:ALA:HA	1:A:399:GLY:O	2.04	0.56
1:A:192:MET:HB2	9:A:607:HOH:O	2.04	0.56
1:A:477:LEU:CD1	5:A:800:HEM:HMB3	2.35	0.56
1:A:221:PRO:HB2	2:B:128:LEU:HD23	1.88	0.56
1:A:267:LEU:CD1	9:A:618:HOH:O	2.53	0.56
1:A:12:TYR:HB3	1:A:19:LYS:HD3	1.88	0.56
1:A:48:ASN:HD21	1:A:457:PRO:HA	1.71	0.56
1:A:207:PHE:HB3	1:A:219:VAL:HG13	1.87	0.56
1:A:449:ARG:NH1	6:A:801:HAS:O2A	2.38	0.55
1:A:499:PRO:HB3	1:A:502:ALA:CB	2.34	0.55
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.37	0.55
1:A:506:LEU:O	1:A:508:PHE:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:VAL:CG2	9:A:621:HOH:O	2.50	0.55
1:A:410:GLY:CA	1:A:502:ALA:HB2	2.35	0.55
1:A:47:GLY:HA3	1:A:471:VAL:HG23	1.89	0.54
1:A:366:ASN:HB3	6:A:801:HAS:HMD	1.89	0.54
2:B:149:CYS:C	9:B:181:HOH:O	2.50	0.54
3:C:10:ALA:O	3:C:14:VAL:HG23	2.08	0.54
1:A:106:MET:HA	1:A:162:ILE:HD11	1.91	0.53
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.43	0.53
1:A:9:SER:C	1:A:11:VAL:N	2.66	0.53
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.09	0.53
1:A:364:ILE:HD12	3:C:19:ILE:HD13	1.91	0.53
1:A:465:VAL:HG13	9:A:604:HOH:O	2.08	0.52
1:A:486:TYR:CG	1:A:486:TYR:O	2.62	0.52
1:A:515:PRO:HD3	2:B:5:HIS:NE2	2.24	0.52
1:A:518:ARG:HD2	9:A:605:HOH:O	2.09	0.52
2:B:4:GLN:O	2:B:4:GLN:HG3	2.08	0.52
2:B:150:ASN:HB3	9:B:181:HOH:O	2.10	0.52
1:A:160:ILE:CD1	1:A:194:PHE:HB2	2.40	0.52
1:A:485:ILE:C	1:A:487:GLY:H	2.18	0.52
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.44	0.52
2:B:74:THR:HG22	2:B:78:GLN:HB3	1.91	0.52
1:A:207:PHE:O	1:A:210:PRO:HD2	2.09	0.51
1:A:157:TRP:HA	1:A:160:ILE:HG13	1.93	0.51
1:A:477:LEU:HD12	5:A:800:HEM:HMB3	1.93	0.51
1:A:412:PRO:HG3	1:A:498:LYS:HB2	1.93	0.51
1:A:257:GLY:HA3	1:A:323:ALA:HB2	1.92	0.50
1:A:140:LYS:CD	9:A:588:HOH:O	2.59	0.50
1:A:272:PHE:O	1:A:276:SER:HB2	2.11	0.50
1:A:8:ILE:C	1:A:10:ARG:N	2.67	0.50
1:A:136:TYR:HE2	9:A:568:HOH:O	1.95	0.50
1:A:89:MET:HE1	1:A:245:ALA:HB2	1.94	0.50
1:A:455:GLN:C	1:A:457:PRO:HD3	2.37	0.50
2:B:12:LEU:HD13	9:B:173:HOH:O	2.12	0.50
1:A:70:THR:HA	9:A:582:HOH:O	2.12	0.50
1:A:89:MET:HB3	1:A:190:TRP:NE1	2.26	0.50
1:A:518:ARG:CG	1:A:518:ARG:HH21	2.24	0.50
1:A:518:ARG:O	1:A:522:LEU:HB2	2.11	0.50
1:A:401:LEU:O	1:A:405:LEU:HB2	2.12	0.49
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.47	0.49
1:A:207:PHE:HB3	1:A:219:VAL:CG1	2.42	0.49
1:A:89:MET:HB3	1:A:190:TRP:HE1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLY:HA3	9:A:575:HOH:O	2.12	0.49
1:A:156:THR:O	1:A:160:ILE:HG13	2.12	0.49
1:A:86:GLN:NE2	1:A:155:SER:HB3	2.24	0.49
1:A:17:GLU:OE1	1:A:100:ARG:HD3	2.12	0.49
1:A:90:VAL:O	1:A:93:PRO:HD2	2.13	0.49
2:B:50:LEU:HD22	2:B:52:ARG:NE	2.28	0.49
2:B:29:PHE:HZ	3:C:20:LEU:HD23	1.77	0.48
2:B:74:THR:HG23	2:B:78:GLN:OE1	2.12	0.48
2:B:55:PRO:O	2:B:58:VAL:HG12	2.13	0.48
1:A:446:ASN:ND2	2:B:117:HIS:CE1	2.82	0.48
1:A:106:MET:HA	1:A:162:ILE:CD1	2.44	0.48
1:A:125:LEU:CB	9:A:578:HOH:O	2.61	0.48
1:A:239:TRP:HE3	6:A:801:HAS:HBC2	1.77	0.48
1:A:520:LEU:HB3	9:A:617:HOH:O	2.06	0.47
1:A:8:ILE:C	1:A:10:ARG:H	2.22	0.47
1:A:537:LEU:HA	1:A:537:LEU:HD23	1.70	0.47
1:A:458:ASP:HB2	9:A:590:HOH:O	2.13	0.47
2:B:33:ILE:O	2:B:36:THR:N	2.46	0.47
1:A:402:TYR:N	1:A:402:TYR:HD2	2.13	0.47
2:B:149:CYS:HB3	2:B:160:MET:HB3	1.96	0.47
1:A:527:ILE:HG22	1:A:528:GLY:N	2.29	0.47
1:A:389:VAL:CB	9:A:621:HOH:O	2.62	0.47
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.98	0.46
1:A:104:GLY:CA	7:A:805:BNG:H4	2.45	0.46
1:A:192:MET:CA	9:A:607:HOH:O	2.63	0.46
1:A:174:ASN:O	1:A:177:LYS:HB2	2.16	0.46
1:A:192:MET:CG	9:A:607:HOH:O	2.63	0.46
1:A:125:LEU:HB3	9:A:578:HOH:O	2.16	0.46
1:A:330:ARG:HB2	1:A:334:GLY:HA3	1.98	0.45
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.52	0.45
1:A:495:ARG:HA	1:A:495:ARG:HD3	1.54	0.45
1:A:134:THR:HG22	1:A:228:PHE:CE2	2.51	0.45
2:B:41:THR:O	2:B:44:VAL:HG22	2.17	0.45
1:A:61:PHE:CE2	1:A:62:VAL:HG23	2.51	0.45
1:A:71:LEU:O	1:A:75:LEU:HB2	2.17	0.45
1:A:134:THR:HG22	1:A:228:PHE:CZ	2.52	0.45
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.98	0.45
1:A:459:ALA:O	2:B:146:ARG:NH1	2.42	0.45
1:A:72:HIS:O	1:A:76:ASN:HB2	2.16	0.45
1:A:8:ILE:HA	1:A:10:ARG:HG3	1.98	0.45
2:B:37:LEU:HA	2:B:42:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:CD2	1:A:233:HIS:C	2.94	0.44
2:B:66:ASP:HA	2:B:67:PRO:HD2	1.69	0.44
1:A:85:ALA:O	1:A:89:MET:HB2	2.18	0.44
1:A:101:PRO:HB3	1:A:166:LEU:HD11	1.99	0.44
1:A:133:TYR:OH	6:A:801:HAS:O1A	2.31	0.44
1:A:189:PHE:CE1	1:A:241:LEU:HB2	2.53	0.44
2:B:12:LEU:O	2:B:12:LEU:HG	2.18	0.44
2:B:37:LEU:HD12	2:B:37:LEU:N	2.33	0.44
1:A:366:ASN:CB	6:A:801:HAS:CMD	2.96	0.44
1:A:386:HIS:CE1	5:A:800:HEM:C1A	3.06	0.44
1:A:262:ASP:OD2	1:A:266:ARG:NE	2.50	0.44
1:A:365:VAL:O	1:A:366:ASN:C	2.61	0.44
1:A:386:HIS:HE1	5:A:800:HEM:C1A	2.36	0.43
1:A:515:PRO:O	1:A:517:ASP:N	2.51	0.43
1:A:192:MET:HA	9:A:607:HOH:O	2.18	0.43
2:B:10:ALA:O	2:B:13:ALA:N	2.41	0.43
1:A:280:GLY:C	9:A:572:HOH:O	2.61	0.43
1:A:90:VAL:C	1:A:93:PRO:HD2	2.44	0.43
1:A:330:ARG:HG3	1:A:330:ARG:NH2	2.17	0.43
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.65	0.43
2:B:44:VAL:CG2	9:B:176:HOH:O	2.66	0.43
2:B:64:TRP:CE2	2:B:82:TYR:HD2	2.35	0.43
2:B:103:ILE:O	2:B:136:ARG:HA	2.18	0.43
1:A:56:LYS:HE2	1:A:60:PRO:O	2.19	0.43
1:A:282:HIS:CD2	1:A:283:HIS:CD2	3.07	0.42
1:A:411:LYS:HE2	1:A:494:SER:O	2.19	0.42
1:A:477:LEU:HD13	5:A:800:HEM:HMB3	2.01	0.42
1:A:7:GLU:HB3	1:A:13:GLU:HG2	2.01	0.42
1:A:35:GLY:HA3	1:A:76:ASN:ND2	2.34	0.42
1:A:307:VAL:HA	1:A:310:LEU:HD12	2.01	0.42
1:A:339:LEU:HB3	1:A:346:PHE:CZ	2.54	0.42
2:B:96:GLU:HA	2:B:165:VAL:O	2.19	0.42
2:B:44:VAL:HG21	9:B:176:HOH:O	2.18	0.42
1:A:56:LYS:O	1:A:56:LYS:HD3	2.20	0.42
1:A:465:VAL:O	1:A:466:PRO:C	2.60	0.42
2:B:58:VAL:HG22	2:B:64:TRP:HB2	2.00	0.42
1:A:23:TYR:HB3	1:A:110:TRP:CD1	2.55	0.42
1:A:282:HIS:HA	1:A:285:PHE:CE1	2.55	0.42
1:A:342:ASP:OD1	1:A:342:ASP:N	2.44	0.42
1:A:12:TYR:CG	1:A:19:LYS:HB2	2.55	0.42
1:A:259:LEU:HD11	9:A:565:HOH:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:801:HAS:HBC2	9:A:621:HOH:O	2.20	0.42
1:A:506:LEU:N	1:A:506:LEU:CD2	2.57	0.42
1:A:225:ARG:HD3	1:A:287:ASP:OD1	2.19	0.41
1:A:182:VAL:O	1:A:185:MET:HB2	2.20	0.41
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.95	0.41
1:A:281:PHE:N	9:A:572:HOH:O	2.53	0.41
1:A:410:GLY:HA3	1:A:499:PRO:CB	2.51	0.41
2:B:117:HIS:HD2	2:B:123:ILE:O	2.03	0.41
1:A:102:ASN:OD1	1:A:105:LEU:N	2.44	0.41
1:A:228:PHE:CG	9:A:568:HOH:O	2.72	0.41
1:A:401:LEU:HD12	1:A:401:LEU:HA	1.88	0.41
1:A:515:PRO:C	1:A:517:ASP:H	2.28	0.41
2:B:146:ARG:HD3	2:B:148:ILE:HD11	2.02	0.41
1:A:274:LEU:N	1:A:274:LEU:CD1	2.83	0.41
1:A:392:LEU:HD12	1:A:392:LEU:HA	1.64	0.41
1:A:386:HIS:HE1	5:A:800:HEM:C4D	2.38	0.41
1:A:225:ARG:NH2	1:A:287:ASP:OD2	2.54	0.41
1:A:152:PHE:O	1:A:155:SER:HB2	2.21	0.41
1:A:196:ALA:HB1	1:A:234:PRO:HG2	2.02	0.41
1:A:281:PHE:H	1:A:298:HIS:CD2	2.36	0.41
1:A:344:PRO:HG2	1:A:402:TYR:CD1	2.56	0.41
1:A:405:LEU:O	1:A:406:PRO:C	2.63	0.41
2:B:31:ALA:O	2:B:34:ALA:HB3	2.21	0.41
1:A:343:ASN:O	1:A:347:VAL:HG23	2.21	0.40
1:A:92:LEU:HB3	1:A:182:VAL:HG11	2.03	0.40
1:A:250:ILE:HD12	1:A:403:TRP:CH2	2.56	0.40
1:A:262:ASP:HB3	1:A:263:PRO:CD	2.51	0.40
3:C:3:GLU:HG3	3:C:4:LYS:N	2.36	0.40
1:A:499:PRO:CB	1:A:502:ALA:HB3	2.43	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:CD	9:A:590:HOH:O[4_444]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/618 (90%)	464 (84%)	71 (13%)	20 (4%)	2	10
2	B	164/166 (99%)	146 (89%)	14 (8%)	4 (2%)	4	17
3	C	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
All	All	750/817 (92%)	639 (85%)	87 (12%)	24 (3%)	3	11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	57	ARG
1	A	58	LEU
1	A	330	ARG
1	A	501	LEU
1	A	517	ASP
1	A	518	ARG
2	B	10	ALA
2	B	11	ILE
2	B	87	ALA
2	B	88	PHE
1	A	11	VAL
1	A	87	ALA
1	A	88	ILE
1	A	102	ASN
1	A	127	ASN
1	A	452	TYR
1	A	486	TYR
1	A	516	GLU
1	A	98	ASN
1	A	280	GLY
1	A	68	GLY
1	A	526	ARG
1	A	515	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/503 (90%)	402 (89%)	51 (11%)	5	19
2	B	136/136 (100%)	121 (89%)	15 (11%)	6	20
3	C	26/26 (100%)	24 (92%)	2 (8%)	12	36
All	All	615/665 (92%)	547 (89%)	68 (11%)	6	20

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	13	GLU
1	A	17	GLU
1	A	25	LEU
1	A	54	LEU
1	A	89	MET
1	A	95	ARG
1	A	96	GLU
1	A	122	LEU
1	A	133	TYR
1	A	155	SER
1	A	160	ILE
1	A	168	ARG
1	A	178	VAL
1	A	183	THR
1	A	219	VAL
1	A	230	TRP
1	A	235	ILE
1	A	250	ILE
1	A	274	LEU
1	A	276	SER
1	A	290	ILE
1	A	307	VAL
1	A	309	SER
1	A	315	THR
1	A	326	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	330	ARG
1	A	337	ARG
1	A	339	LEU
1	A	350	VAL
1	A	354	LEU
1	A	370	THR
1	A	371	LEU
1	A	391	SER
1	A	401	LEU
1	A	430	LEU
1	A	435	MET
1	A	439	LEU
1	A	449	ARG
1	A	465	VAL
1	A	467	MET
1	A	472	LEU
1	A	478	LEU
1	A	490	SER
1	A	495	ARG
1	A	506	LEU
1	A	518	ARG
1	A	520	LEU
1	A	522	LEU
1	A	526	ARG
1	A	527	ILE
2	B	6	LYS
2	B	12	LEU
2	B	19	LEU
2	B	23	LEU
2	B	26	LEU
2	B	49	LYS
2	B	74	THR
2	B	78	GLN
2	B	102	GLU
2	B	107	ILE
2	B	140	LYS
2	B	141	ARG
2	B	148	ILE
2	B	166	VAL
2	B	167	LYS
3	C	13	LEU
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	48	ASN
1	A	76	ASN
1	A	82	GLN
1	A	86	GLN
1	A	127	ASN
1	A	254	GLN
1	A	284	GLN
1	A	298	HIS
1	A	388	GLN
1	A	446	ASN
1	A	554	ASN
2	B	4	GLN
2	B	69	GLN
2	B	91	GLN
2	B	117	HIS
2	B	122	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	BNG	A	806	-	21,21,21	1.03	1 (4%)	26,26,26	1.17	3 (11%)
6	HAS	A	801	1	72,72,72	2.45	24 (33%)	87,109,109	2.57	30 (34%)
7	BNG	A	805	-	21,21,21	0.83	1 (4%)	26,26,26	1.02	0
7	BNG	C	804	-	21,21,21	0.83	1 (4%)	26,26,26	1.43	6 (23%)
8	CUA	B	802	2	0,1,1	-	-	-	-	-
7	BNG	A	807	-	21,21,21	0.68	1 (4%)	26,26,26	1.23	4 (15%)
5	HEM	A	800	1	50,50,50	2.20	9 (18%)	67,82,82	1.86	18 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BNG	A	806	-	-	9/12/32/32	0/1/1/1
6	HAS	A	801	1	1/1/8/18	5/42/82/82	-
7	BNG	A	805	-	-	8/12/32/32	0/1/1/1
7	BNG	C	804	-	-	7/12/32/32	0/1/1/1
7	BNG	A	807	-	-	9/12/32/32	0/1/1/1
5	HEM	A	800	1	-	5/14/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3D-C2D	9.02	1.56	1.36
5	A	800	HEM	FE-NB	6.05	2.13	1.94
6	A	801	HAS	FE-NA	5.37	2.12	1.95
6	A	801	HAS	CHB-C1D	5.23	1.49	1.38
6	A	801	HAS	C2A-C3A	5.05	1.47	1.36
6	A	801	HAS	FE-ND	5.01	2.10	1.94
6	A	801	HAS	CHA-C1A	4.95	1.48	1.38
6	A	801	HAS	FE-NB	4.91	2.10	1.94
6	A	801	HAS	FE-NC	4.83	2.11	1.95
5	A	800	HEM	FE-NA	4.78	2.10	1.95
5	A	800	HEM	CMB-C2B	4.74	1.60	1.50
6	A	801	HAS	C2D-C3D	4.57	1.47	1.37
6	A	801	HAS	CHC-C1C	4.43	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	CHA-C4D	4.36	1.49	1.39
6	A	801	HAS	CHC-C4B	4.28	1.47	1.38
6	A	801	HAS	CHD-C4A	4.24	1.46	1.38
6	A	801	HAS	CAC-C3C	-4.22	1.36	1.47
6	A	801	HAS	C11-C3B	-4.11	1.46	1.51
6	A	801	HAS	CHB-C1B	3.82	1.47	1.39
5	A	800	HEM	CMC-C2C	3.37	1.57	1.50
6	A	801	HAS	CHD-C4C	3.17	1.46	1.39
5	A	800	HEM	CAB-C3B	3.16	1.55	1.47
6	A	801	HAS	C4D-C3D	-3.06	1.39	1.45
7	A	806	BNG	O1-C1	3.03	1.45	1.40
6	A	801	HAS	C1D-ND	-2.75	1.35	1.40
5	A	800	HEM	CAC-C3C	2.74	1.54	1.47
6	A	801	HAS	C4B-C3B	-2.69	1.40	1.44
7	C	804	BNG	O1-C1	2.64	1.44	1.40
6	A	801	HAS	C2D-C1D	-2.62	1.39	1.44
6	A	801	HAS	C4A-C3A	2.57	1.50	1.45
6	A	801	HAS	CMD-C2D	2.55	1.51	1.45
6	A	801	HAS	C1A-C2A	2.43	1.49	1.45
7	A	805	BNG	O1-C1	2.39	1.44	1.40
5	A	800	HEM	CAA-C2A	2.30	1.57	1.51
5	A	800	HEM	C4D-ND	2.26	1.44	1.40
7	A	807	BNG	O1-C1	2.25	1.44	1.40
6	A	801	HAS	C4A-NA	-2.06	1.35	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CBC-CAC-C3C	8.71	171.03	127.53
6	A	801	HAS	CMC-C2C-C1C	6.88	135.89	125.42
6	A	801	HAS	C2D-C3D-C4D	-5.87	102.18	106.43
6	A	801	HAS	C2A-C1A-NA	5.83	115.95	110.32
5	A	800	HEM	C4D-ND-C1D	5.66	111.91	105.21
6	A	801	HAS	C3C-C2C-C1C	-4.85	101.46	107.17
5	A	800	HEM	CMA-C3A-C4A	-4.81	118.10	125.42
6	A	801	HAS	C3D-C4D-ND	4.71	114.91	110.35
6	A	801	HAS	O11-C11-C3B	-4.41	103.16	111.26
6	A	801	HAS	C2C-C1C-NC	4.35	117.12	110.14
6	A	801	HAS	CAA-CBA-CGA	-4.35	102.12	113.67
5	A	800	HEM	CHA-C4D-ND	4.34	129.74	124.37
6	A	801	HAS	C2B-C1B-NB	4.22	114.78	109.90
5	A	800	HEM	CHD-C4C-NC	4.22	129.04	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CAD-CBD-CGD	-3.96	103.16	113.67
5	A	800	HEM	C4B-C3B-C2B	3.83	110.80	107.28
6	A	801	HAS	C32-C30-C31	3.81	123.37	114.59
6	A	801	HAS	C3A-C4A-NA	3.80	116.67	109.64
6	A	801	HAS	C3B-C4B-NB	3.75	114.15	109.84
6	A	801	HAS	C4B-NB-C1B	-3.67	100.86	105.21
5	A	800	HEM	CMA-C3A-C2A	3.62	133.30	125.62
6	A	801	HAS	O11-C11-C12	3.43	118.22	109.14
7	A	806	BNG	C1-C2-C3	3.37	117.10	110.01
6	A	801	HAS	CHA-C1A-C2A	-3.33	119.61	124.86
6	A	801	HAS	CHB-C1B-NB	-3.32	120.86	124.42
6	A	801	HAS	C4A-C3A-C2A	-3.23	102.19	106.97
7	C	804	BNG	C3-C4-C5	3.17	115.98	110.23
6	A	801	HAS	C1A-C2A-C3A	-3.17	102.94	107.11
7	A	807	BNG	O5-C5-C4	3.15	115.38	109.70
6	A	801	HAS	CAD-C3D-C4D	3.12	130.13	124.70
6	A	801	HAS	C12-C11-C3B	-3.07	107.32	112.12
6	A	801	HAS	CHC-C4B-NB	-2.86	120.83	124.37
6	A	801	HAS	CHD-C4A-C3A	-2.72	119.84	125.49
7	C	804	BNG	C4-C3-C2	2.71	115.58	110.83
5	A	800	HEM	CHC-C1C-NC	2.65	127.33	124.45
6	A	801	HAS	C26-C15-C16	2.54	119.63	115.23
5	A	800	HEM	O2D-CGD-CBD	2.47	121.81	114.00
6	A	801	HAS	CMB-C2B-C1B	2.46	128.87	125.03
7	A	806	BNG	O3-C3-C4	2.39	116.00	110.38
5	A	800	HEM	CAD-C3D-C2D	2.36	132.29	127.87
7	A	807	BNG	O6-C6-C5	-2.36	103.30	111.33
5	A	800	HEM	C4C-CHD-C1D	-2.35	121.03	126.02
5	A	800	HEM	CHD-C1D-ND	2.34	126.94	124.42
7	C	804	BNG	O5-C5-C4	2.34	113.92	109.70
7	C	804	BNG	O5-C1-C2	-2.32	105.60	110.37
5	A	800	HEM	C3B-C4B-NB	-2.31	107.81	109.47
7	A	807	BNG	C4-C3-C2	2.30	114.86	110.83
5	A	800	HEM	CMB-C2B-C1B	2.28	128.60	125.03
6	A	801	HAS	C31-C30-C29	-2.28	115.81	122.66
5	A	800	HEM	C4C-C3C-C2C	2.28	108.79	106.81
6	A	801	HAS	O1A-CGA-CBA	-2.28	115.86	123.09
6	A	801	HAS	C4A-NA-C1A	-2.20	102.24	105.82
7	C	804	BNG	C6-C5-C4	-2.19	107.63	113.02
5	A	800	HEM	CAC-C3C-C4C	-2.18	119.61	124.82
6	A	801	HAS	CHC-C1C-C2C	-2.16	121.15	127.43
5	A	800	HEM	CAA-C2A-C3A	2.15	131.88	127.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	CHA-C4D-C3D	-2.14	121.27	125.23
7	A	807	BNG	C6-C5-C4	-2.14	107.78	113.02
5	A	800	HEM	CHC-C4B-NB	2.11	126.69	124.42
7	C	804	BNG	C1'-O1-C1	2.09	117.25	113.68
7	A	806	BNG	O2-C2-C1	-2.05	105.20	110.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	HAS	NA

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	HAS	C1D-C2D-CMD-OMD
6	A	801	HAS	C3D-C2D-CMD-OMD
7	A	806	BNG	C2'-C1'-O1-C1
7	C	804	BNG	O5-C1-O1-C1'
7	A	806	BNG	O5-C1-O1-C1'
7	A	806	BNG	C2-C1-O1-C1'
7	C	804	BNG	C2-C1-O1-C1'
7	A	807	BNG	C4-C5-C6-O6
7	A	807	BNG	O1-C1'-C2'-C3'
7	A	805	BNG	C2'-C3'-C4'-C5'
7	A	806	BNG	C3'-C4'-C5'-C6'
7	A	807	BNG	C5'-C6'-C7'-C8'
7	A	807	BNG	C1'-C2'-C3'-C4'
7	A	807	BNG	O5-C5-C6-O6
7	A	805	BNG	C5'-C6'-C7'-C8'
7	A	805	BNG	C4'-C5'-C6'-C7'
7	A	806	BNG	O1-C1'-C2'-C3'
7	C	804	BNG	C4-C5-C6-O6
7	C	804	BNG	C1'-C2'-C3'-C4'
7	A	807	BNG	C2'-C3'-C4'-C5'
7	A	807	BNG	C6'-C7'-C8'-C9'
7	A	807	BNG	C2'-C1'-O1-C1
7	A	805	BNG	C3'-C4'-C5'-C6'
7	A	806	BNG	C6'-C7'-C8'-C9'
7	A	805	BNG	C6'-C7'-C8'-C9'
5	A	800	HEM	C2B-C3B-CAB-CBB
5	A	800	HEM	C4B-C3B-CAB-CBB
7	A	806	BNG	C4'-C5'-C6'-C7'

Continued on next page...

Continued from previous page...

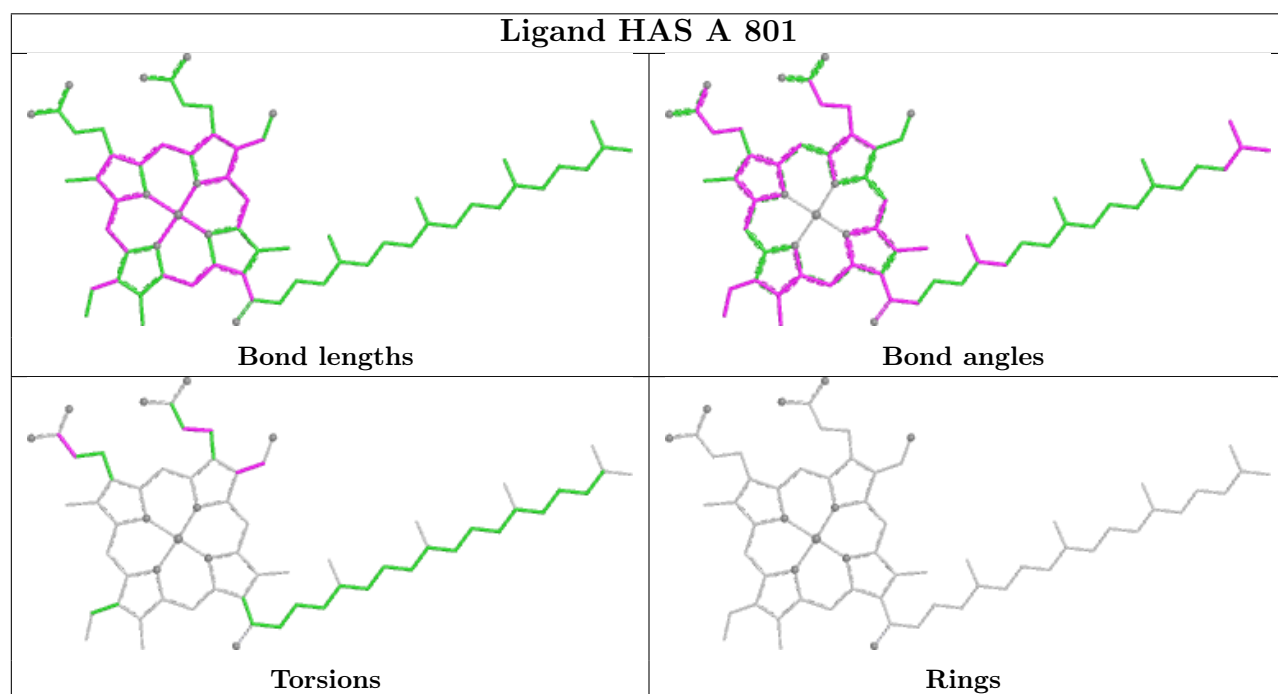
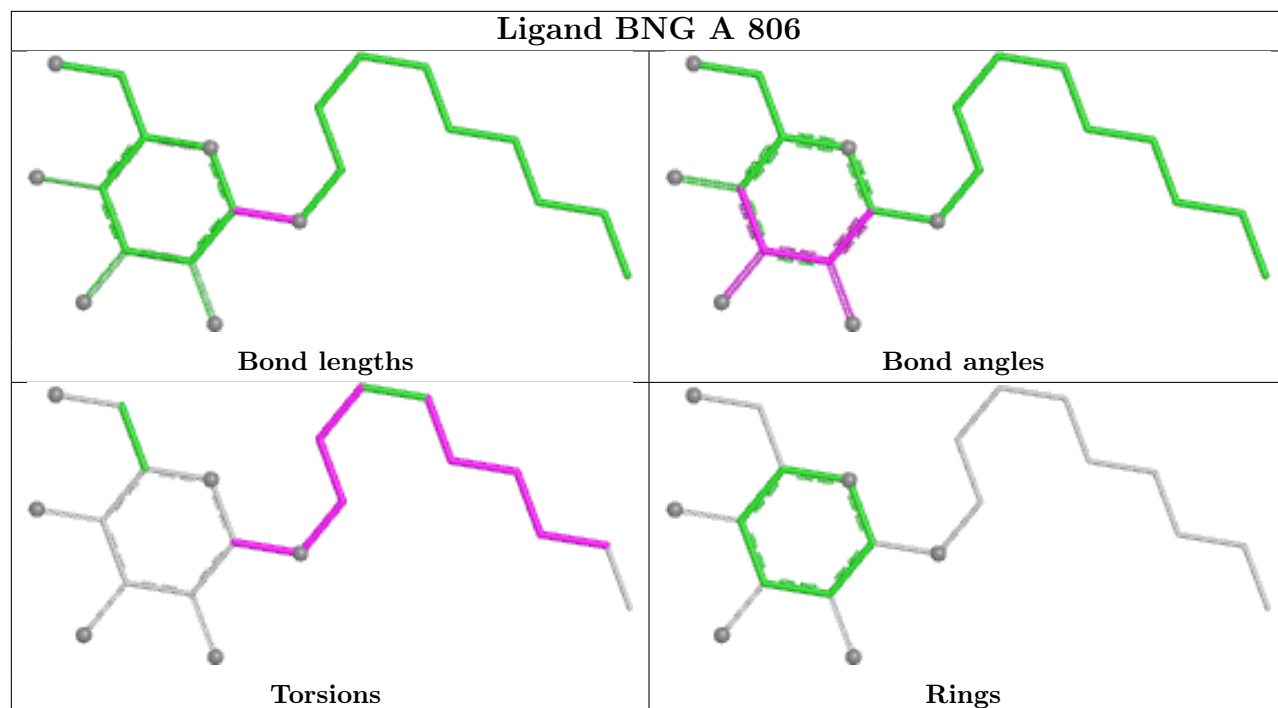
Mol	Chain	Res	Type	Atoms
7	A	806	BNG	C5'-C6'-C7'-C8'
7	C	804	BNG	O1-C1'-C2'-C3'
7	A	805	BNG	C2-C1-O1-C1'
7	A	805	BNG	O1-C1'-C2'-C3'
5	A	800	HEM	C2D-C3D-CAD-CBD
7	A	806	BNG	C1'-C2'-C3'-C4'
5	A	800	HEM	C4D-C3D-CAD-CBD
6	A	801	HAS	CAA-CBA-CGA-O2A
6	A	801	HAS	CAA-CBA-CGA-O1A
7	C	804	BNG	O5-C5-C6-O6
7	A	805	BNG	O5-C1-O1-C1'
7	A	807	BNG	O5-C1-O1-C1'
5	A	800	HEM	CAD-CBD-CGD-O2D
7	C	804	BNG	C5'-C6'-C7'-C8'
6	A	801	HAS	C3D-CAD-CBD-CGD

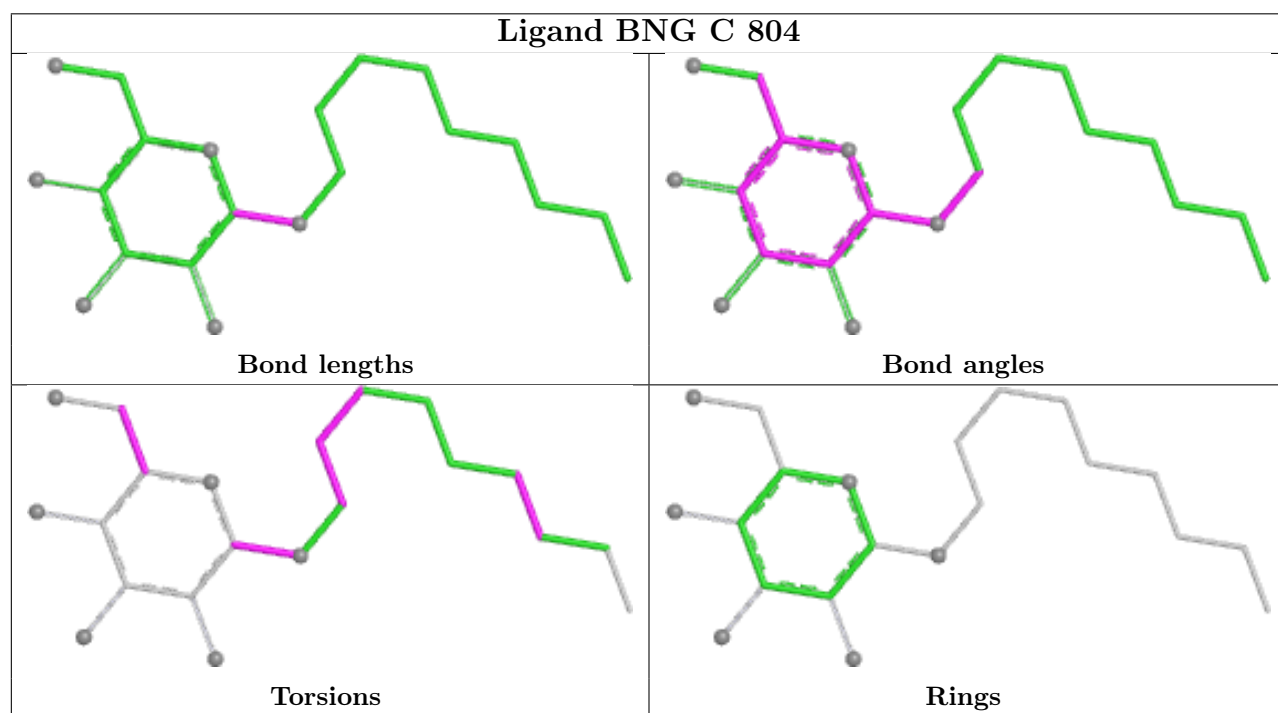
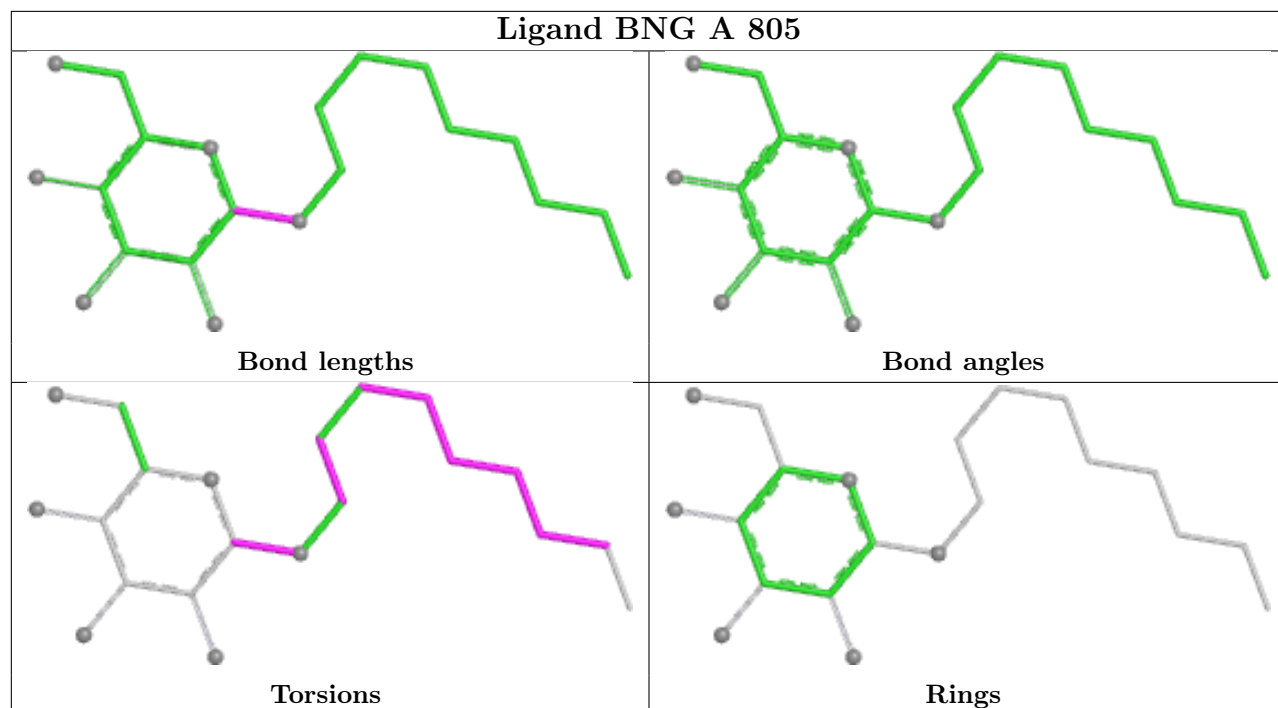
There are no ring outliers.

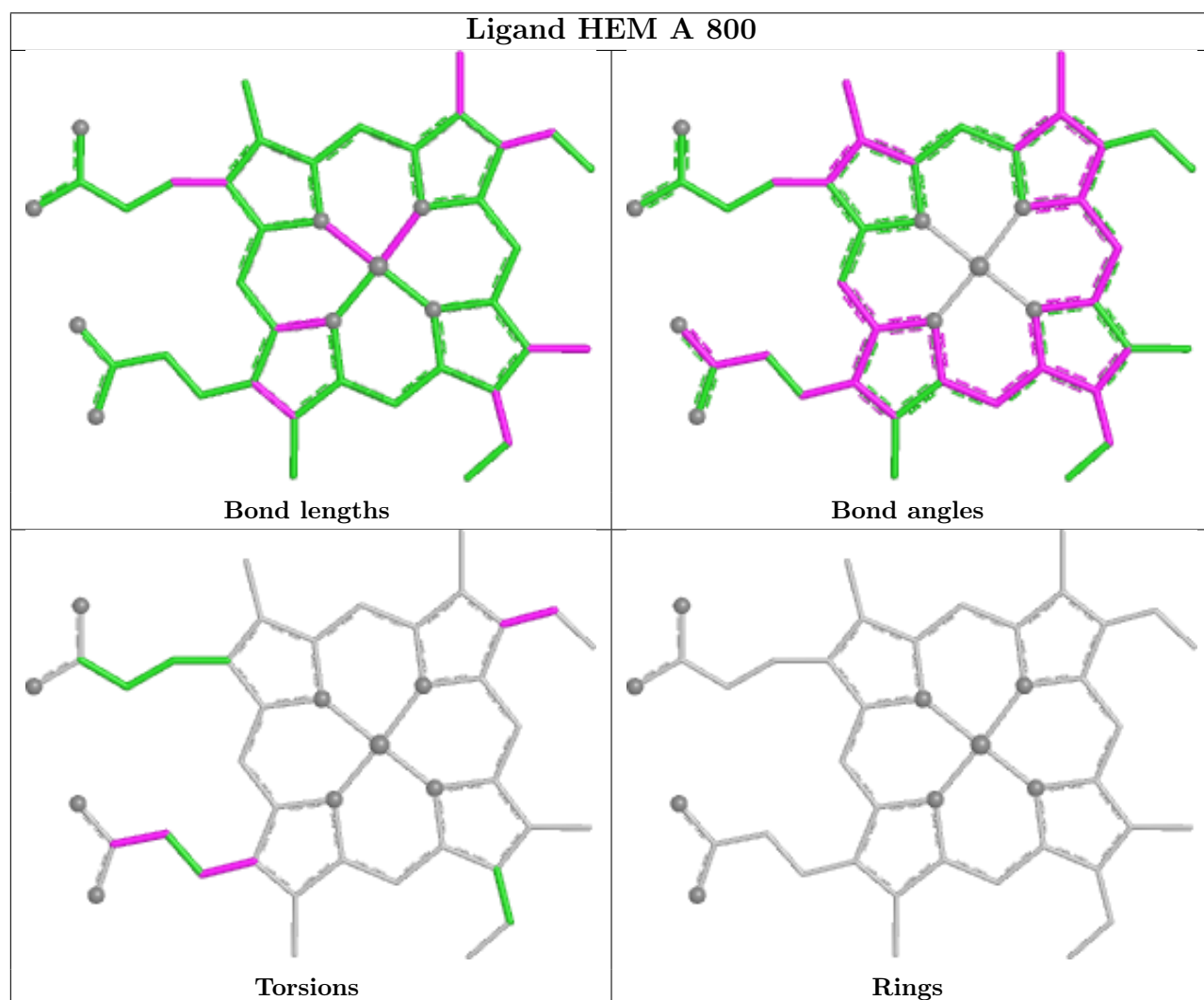
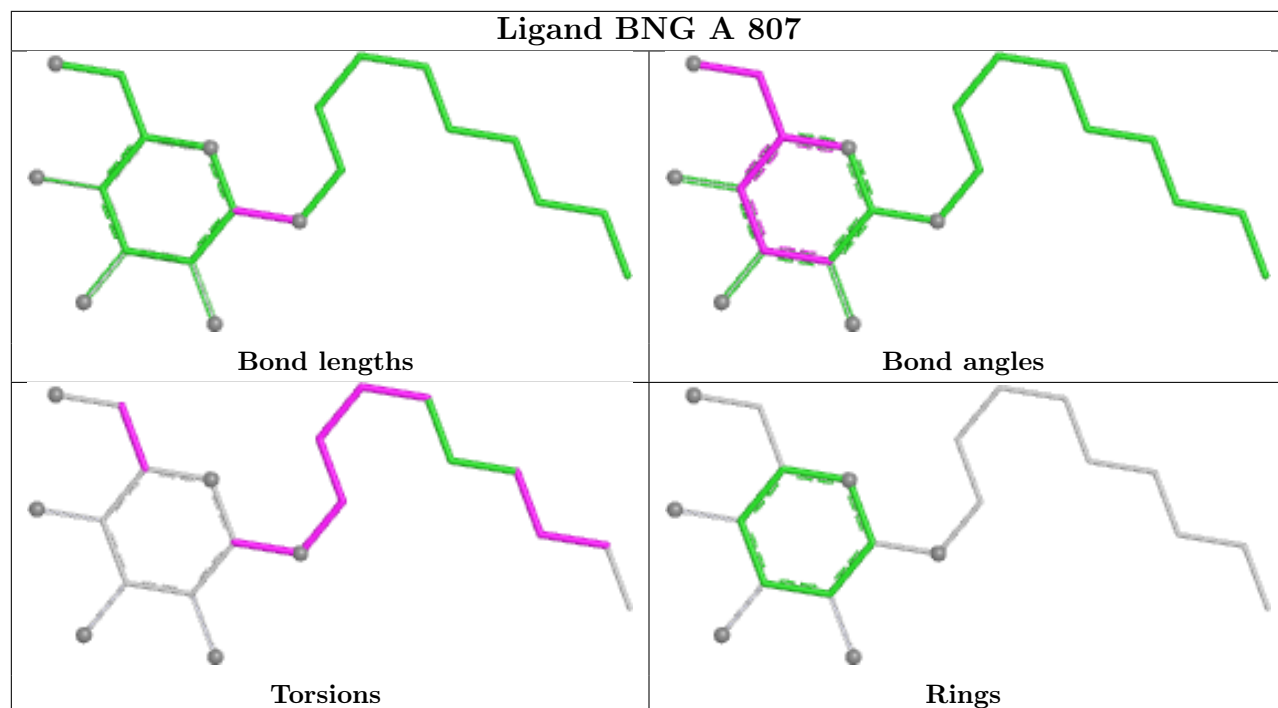
3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	801	HAS	9	0
7	A	805	BNG	2	0
5	A	800	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/618 (90%)	-0.04	15 (2%) 56 46	63, 85, 124, 190	0
2	B	166/166 (100%)	-0.03	2 (1%) 76 68	66, 85, 118, 160	0
3	C	33/33 (100%)	-0.26	1 (3%) 52 42	67, 77, 125, 144	0
All	All	756/817 (92%)	-0.05	18 (2%) 59 49	63, 85, 126, 190	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ILE	3.9
1	A	495	ARG	3.0
1	A	218	GLY	2.9
1	A	178	VAL	2.8
1	A	502	ALA	2.6
1	A	528	GLY	2.5
1	A	515	PRO	2.4
1	A	15	TYR	2.4
1	A	330	ARG	2.3
2	B	69	GLN	2.3
1	A	87	ALA	2.3
1	A	501	LEU	2.3
1	A	503	GLU	2.2
1	A	514	GLY	2.2
1	A	12	TYR	2.1
3	C	34	GLY	2.1
1	A	103	MET	2.1
2	B	10	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

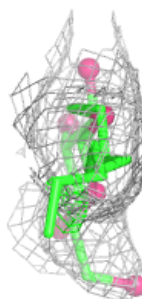
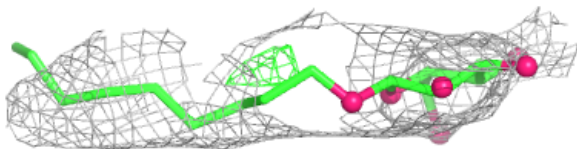
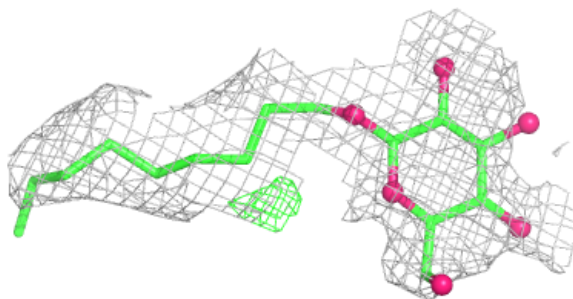
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BNG	A	805	21/21	0.57	0.15	146,158,162,163	0
7	BNG	A	806	21/21	0.63	0.14	134,141,143,144	0
7	BNG	A	807	21/21	0.68	0.16	120,150,158,159	0
7	BNG	C	804	21/21	0.76	0.14	89,134,146,146	0
6	HAS	A	801	65/65	0.95	0.09	58,66,77,83	0
5	HEM	A	800	43/43	0.98	0.07	56,62,74,79	0
8	CUA	B	802	2/2	0.98	0.04	80,80,80,80	0
4	CU1	A	803	1/1	0.99	0.05	80,80,80,80	0

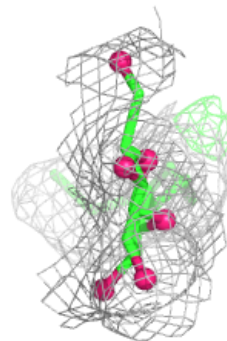
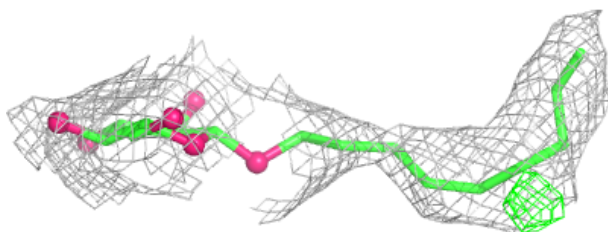
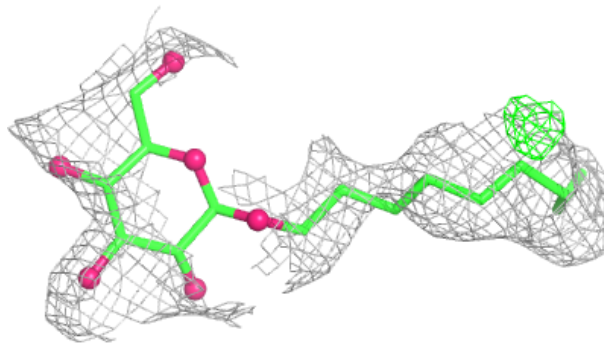
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BNG A 805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

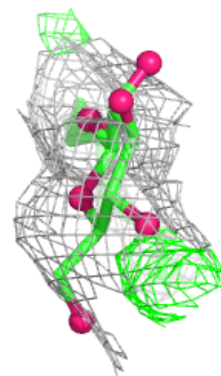
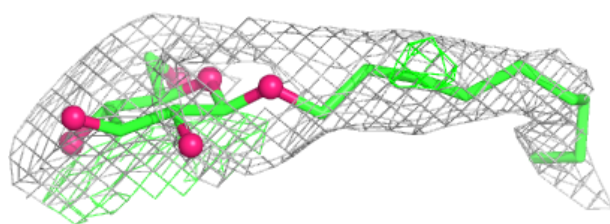
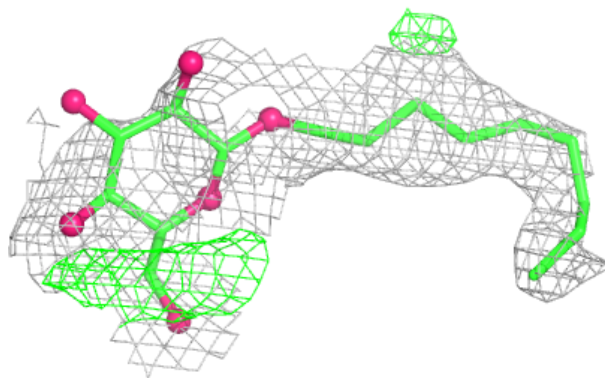
**Electron density around BNG A 806:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

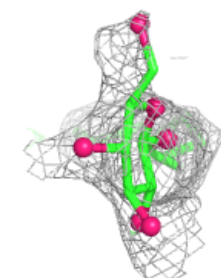
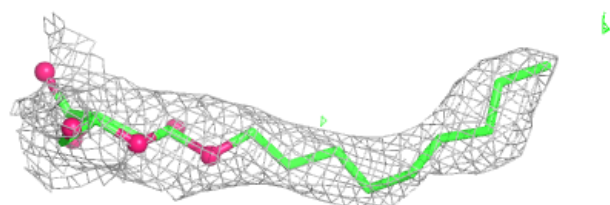


Electron density around BNG A 807:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

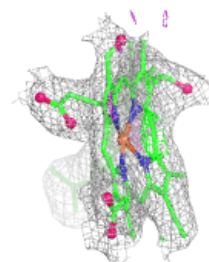
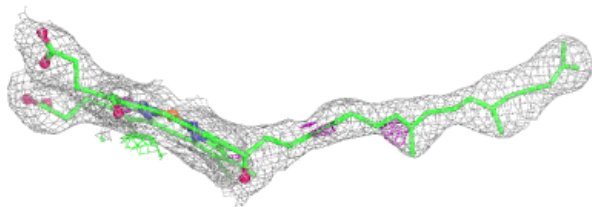
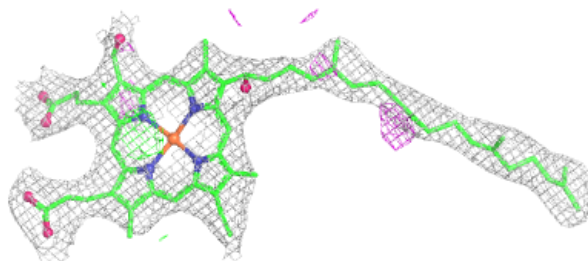
**Electron density around BNG C 804:**

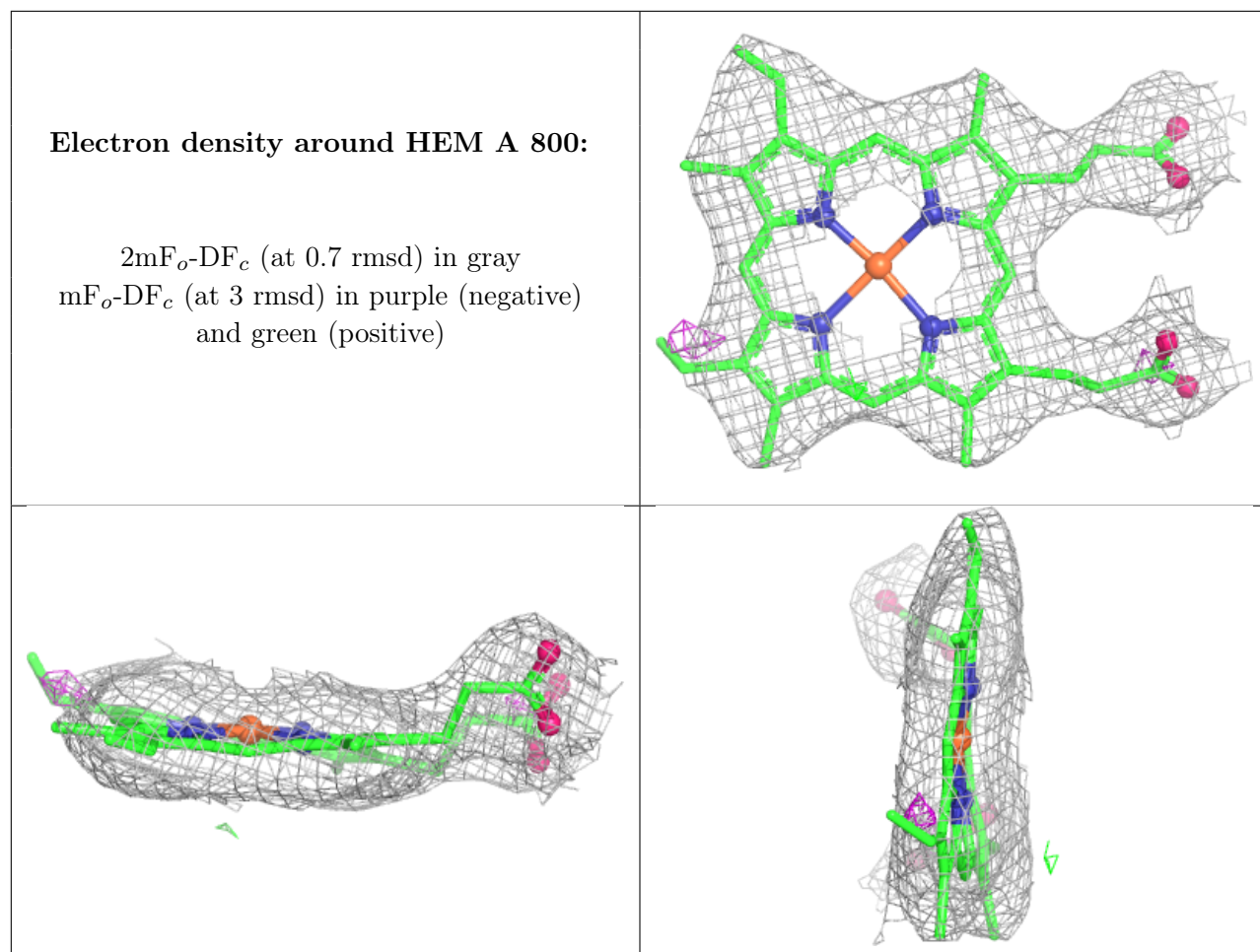
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HAS A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.